Plasma/wall interactions: relevance to BOUT++ simulations and how they can be incorporated

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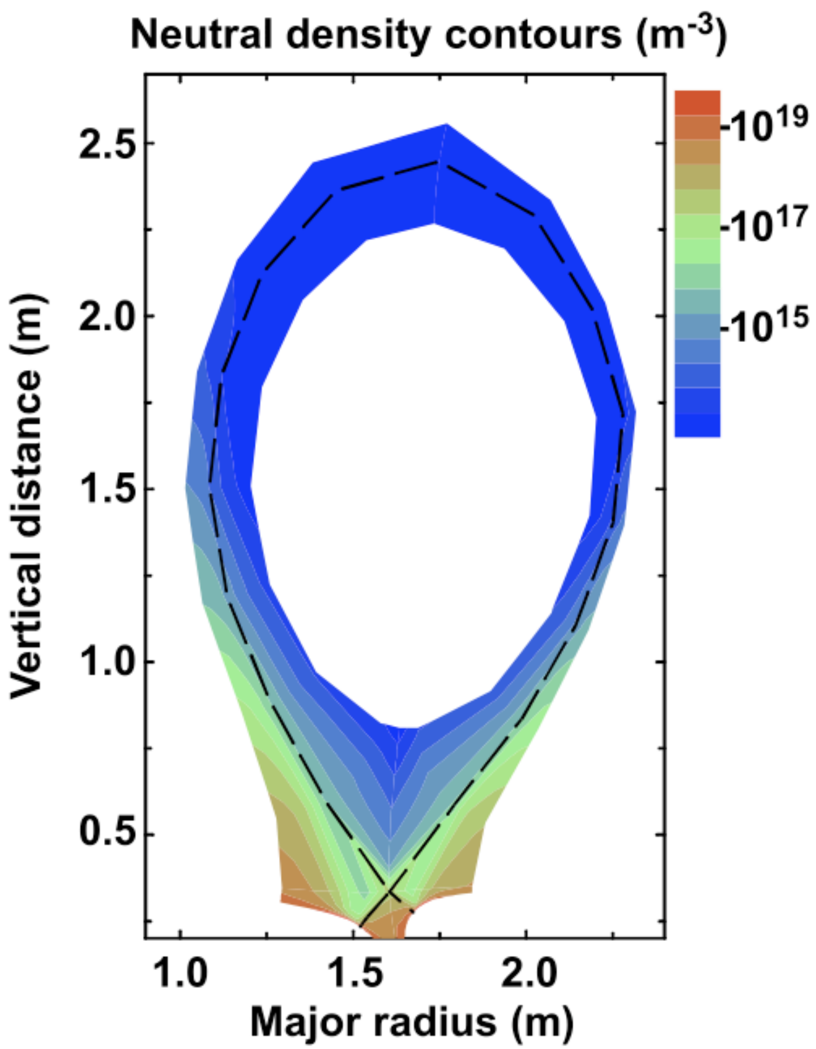
Topics covered

- **Components added by plasma/wall interactions (PWI)**
  1. **Hydrogenic neutrals from plasma recycling and/or injection**
  2. **Impurities from sputtering and/or injection**
  3. **Material damage**
- **Temporal and spatial scales**
  1. **Neutrals**
  2. **Impurities**
  3. **Implications for Turbulence and Transport**
- **Implementable models for neutrals & impurities -> DISCUSSION**

1. Large plasma fluxes saturate materials with neutrals, leading to a large recycling neutral source

- **Neutral flux into the plasma is $\Gamma_n = -R\Gamma_i$, with R ~ 1**
- **Ionization strongly attenuates neutrals –> large gradients**
- **Neutral ionization provides plasma source in SOL and at least in outer pedestal -> needed for profile evolution**
- **Thermal heating of material can cause R(t) > 1 and thus outgassing (e.g., during ELMs [Pigarov])**



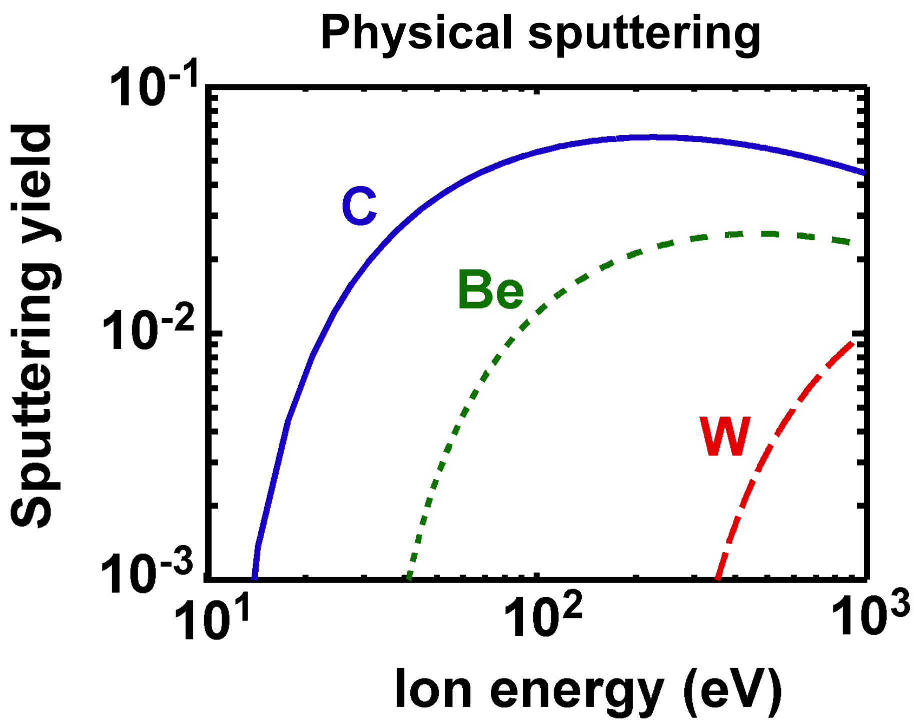
2. Ion sputtering or gas puffing add impurities: radiates exhaust power & can contaminate core

- **Ion sputtering is highly energy and material dependent**

- **Thermal force processes along the magnetic field owing to gradients in T_e and T_i retard impurity intrusion to the midplane**

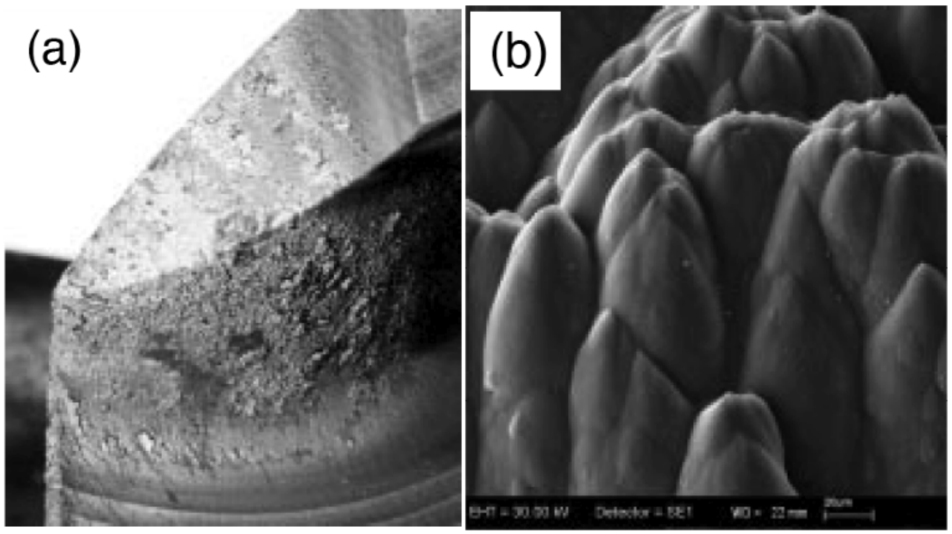
- **Neoclassical pinch process can transport impurities to core; ELMs help expel impurities**

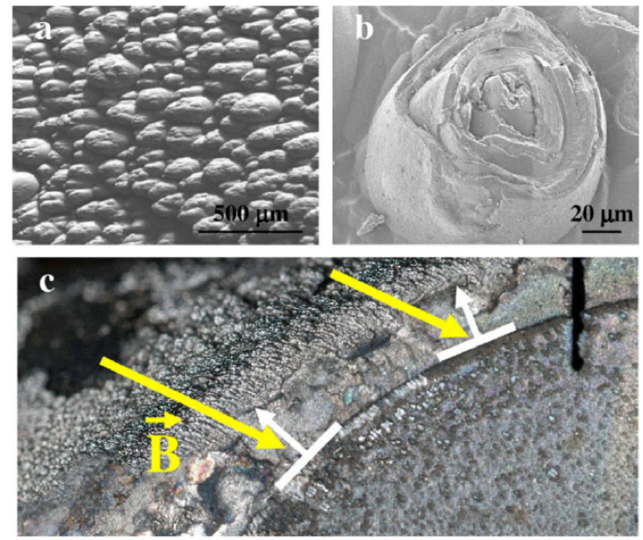
- **Issue: number of impurity charge-states to evolve can be large**



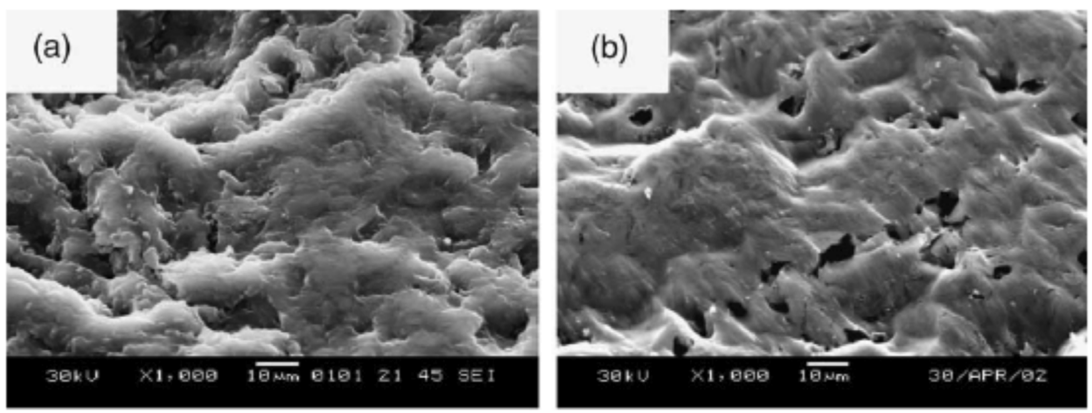
3. Sputtering can modify materials surfaces; BOUT++ could evaluate toroidal asymmetries, but beyond this talk

- **Experimental images of PFC surfaces:**
  - **Images from Tore-Supra, TEXTOR, and LHD: micron size**





From
S. Krasheninnikov,
Sherwood 2013



Neutrals and impurities add various time/space scales

Time scales for plasma/neutral processes are driven by charge exchange and ionization rates

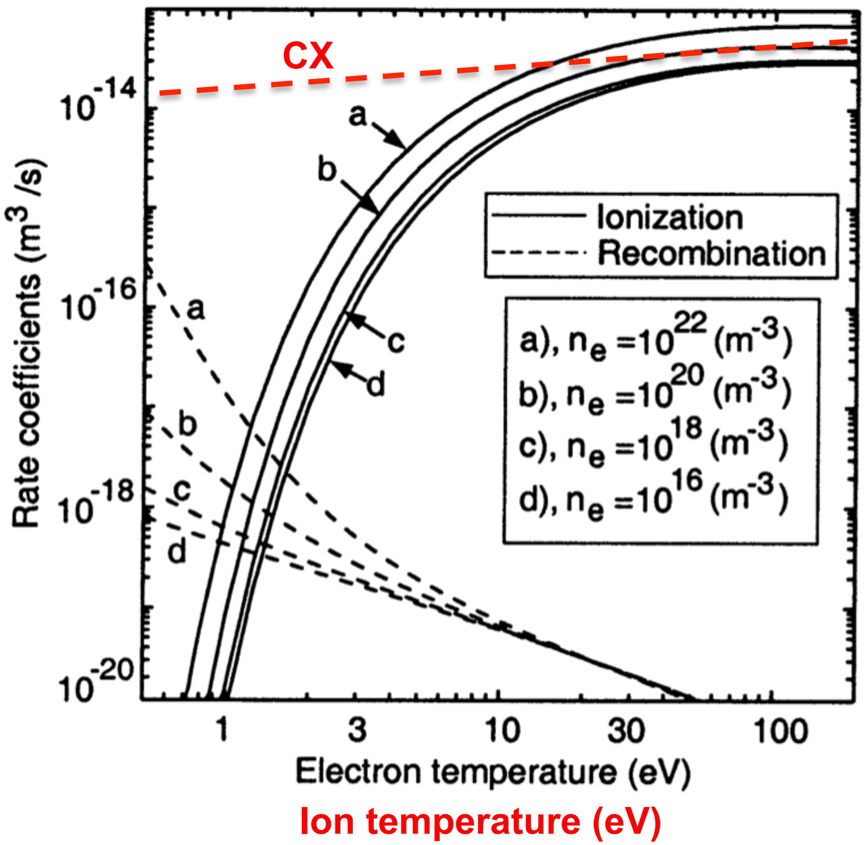
- **Continuity equations describe interaction**
  $$dn_i/dt = -K^i n_e n_g + K^r n_e n_i$$

  as well as momentum exchange
  $$m_i d(n_i v_i)/dt = m_i n_i n_n K^{cx} (v_n - v_i) + \ldots$$

- **Ionization/recombination also gives line-radiation loss from the electron energy channel (T_e)**

- **For hydrogen, CX-collisions dominant neutral motion with diffusion coefficient**
  $$D_g \sim T_g/(m_g K^{cx} n_i)$$
  (which is then flux limited)

Hydrogen rate coeffs.



Typical time/space scales in different regions

- **Midplane separatrix:** $n_i \sim 3\times10^{19}$ m^{-3}, $n_n \sim 10^{16}$ m^{-3}, $T_e \sim$ 50 eV
  - For plasma dynamics, $\nu_{ioniz\text{-}i} = K^i n_n \sim 10^2$ s, $\nu_{cxi} = K^{cx} n_n \sim 10^2$ s
  - For neutral dynamics, $\nu_{ioniz\text{-}n} = K^i n_i \sim 3\times10^5$ s, $\nu_{cxn} = K^{cx} n_i \sim 3\times10^5$ s
  - Radial scale length ~ 1 cm

- **Near divertor plate:** $n_i \sim 3\times10^{20}$ m^{-3}, $n_n \sim 10^{20}$ m^{-3}, $T_e \sim$ 5 eV
  - For plasma dynamics, $\nu_{ioniz\text{-}i} = K^i n_n \sim 10^6$ s, $\nu_{cxi} = K^{cx} n_n \sim 10^6$ s
  - For neutral dynamics, $\nu_{ioniz\text{-}n} = K^i n_i \sim 3\times10^6$ s, $\nu_{cxn} = K^{cx} n_i \sim 3\times10^6$ s
  - Polodial scale length ~1-3 cm

Instabilities unlikely affected by neutrals near separatrix, but may be affected near the divertor plate - ionization instabilities possible – Duncan, Phys Fluids 14 (1971) 1973.

Impurities can radiate substantial electron energy, but densities are small & thus effect on instabilities small(?)

- **Impurities have multiple charge states**

$$\frac{\partial n_j}{\partial t} + \nabla \cdot (n_j v_j) = K^{i}_{j-1} n_e n_{j-1} - K^{r}_{j} n_e n_j$$
$$- K^{i}_{j} n_e n_j + K^{r}_{j+1} n_e n_{j+1}$$

- **Electron energy loss depends sensitively on T_e**

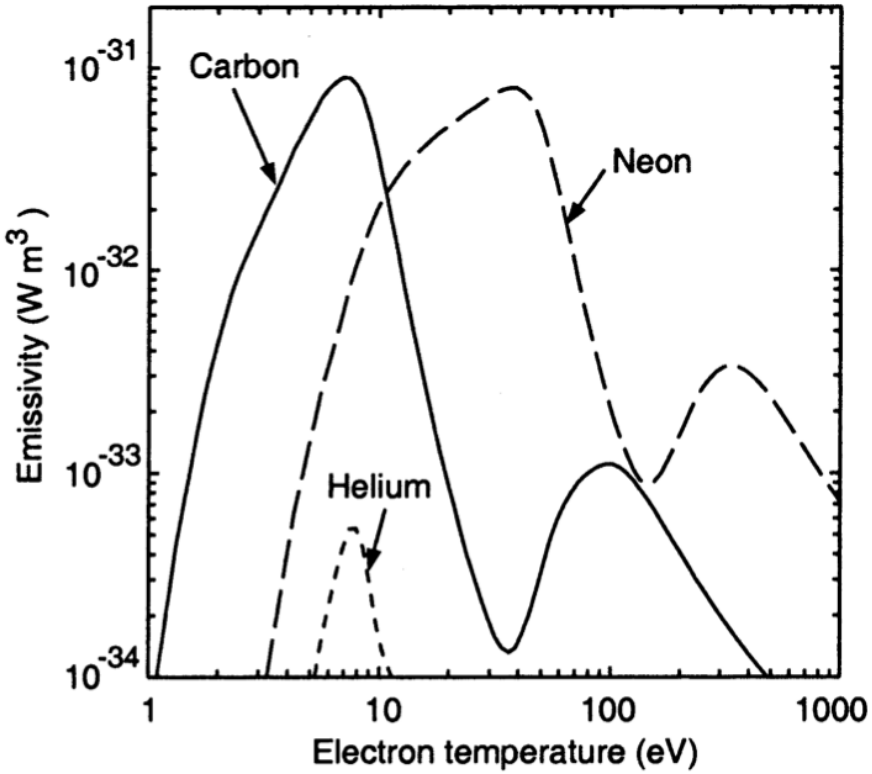
  $d(1.5 n_e T_e)/dt = n_e n_{zt} \varepsilon + \ldots$

- **Gyro-radius & drift motion of impurities vary with charge/mass**

  $\rho_j \sim m_j^{1/2} / Z_j$

  $v\_gradB \sim 1/Z_j$

Emissivity - coronal equilibrium



Impurity effect on microturbulence likely modest unless through T_e eqn. BUT impurity transport can be strongly affected by hydrogen turbulence

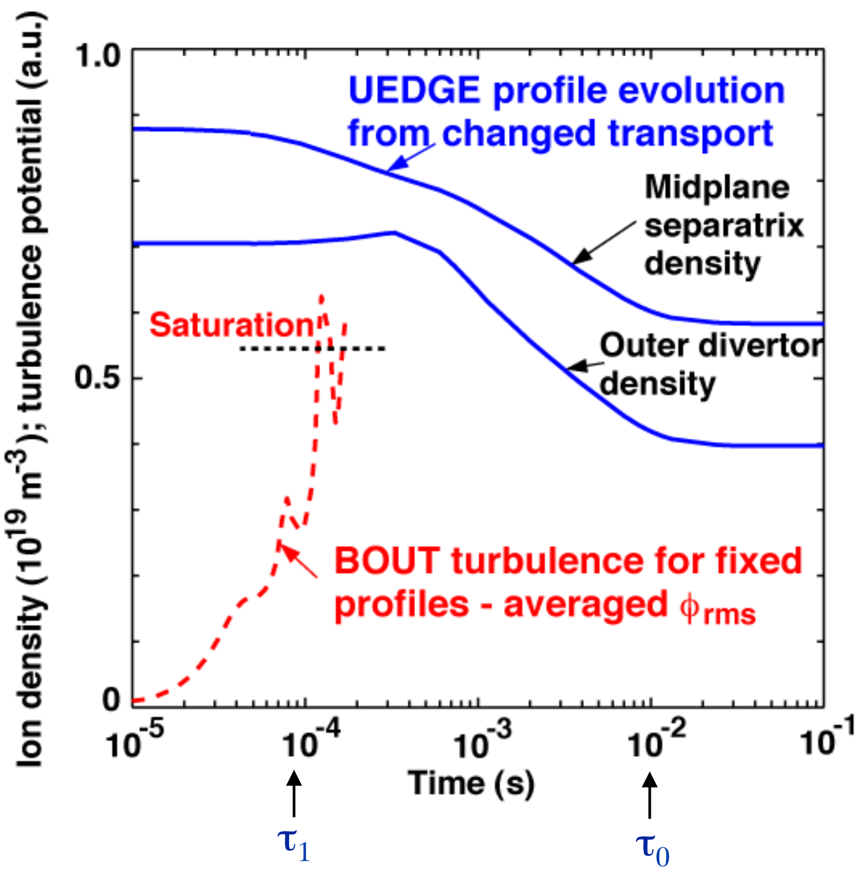
Recycling results in slow SOL transport equilibrium times, whereas turbulence saturation is fast

- **Because R ~ 1, SOL profiles evolve over long time scales (~0.01 s); impurities extend evolution to ~0.1 s**

- **Thus, running BOUT++ to transport equilibrium with neutrals is inefficient**

- **One approach: coupling 3D BOUT turbulence and 2D UEDGE transport via relaxed iterative coupling (RIC; Shestakov, R. Cohen et al.) shown in JNM '05**

Comparison of transport and turbulence timescales



Models for neutrals and impurities –> DISCUSSION

- Atomic rates for ionization/CX/radiation are usually available as simple algebraic fits or table look-usp as a function of n_e and $T_{e,i}$

- Fluid models can use existing discretization/solution-techniques in BOUT++; example is Wang et al. (SWIP and LLNL)

- BUT strong preconditioning is likely needed for good numerical performance of neutral fluid if long-time transport is goal (next page)

- Kinetic models offer extended physics capability, but efficient coupling to plasma is a major task (Univ. of York)

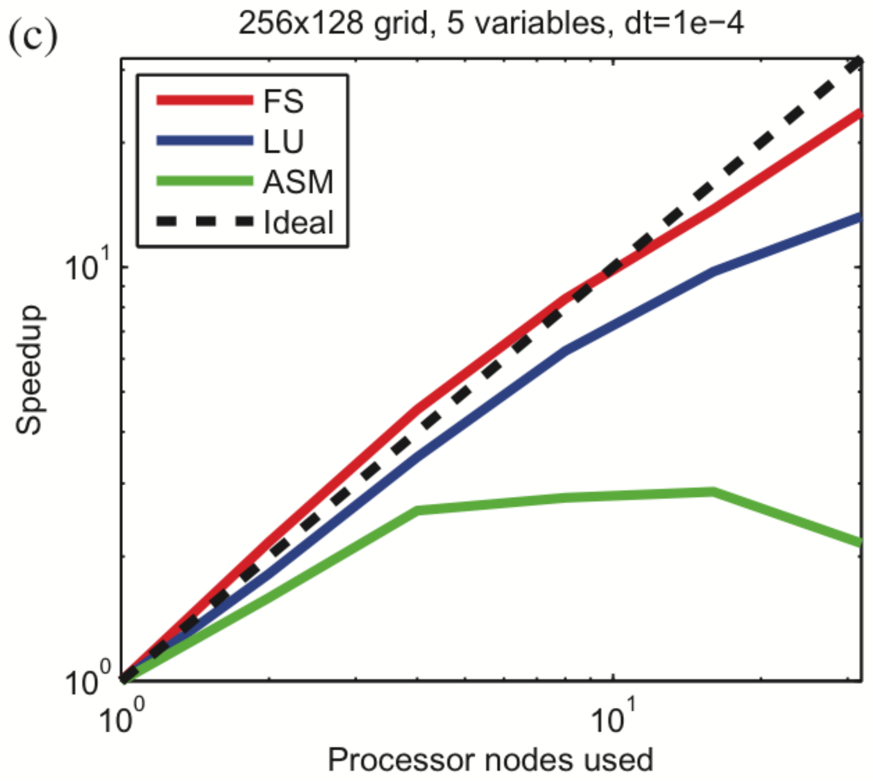
Issue: fluid neutral model need strong preconditioner for efficiency of long-time transport simulations

- **Because neutral fluid transport is isotropic, its performance is sensitive to the anisotropic mesh, especially in domain-decomposed parallel applications**

- **During the FACETS SciDAC, a field-split (FS) algorithm was developed to overcome this difficulty by reordering eqn variables and treating neutral preconditioning different [McCourt, Rognlien, McInnes, Zhang, Comp Sci Disc 5 (2012) 014012]**

FS = Field split method

(c)

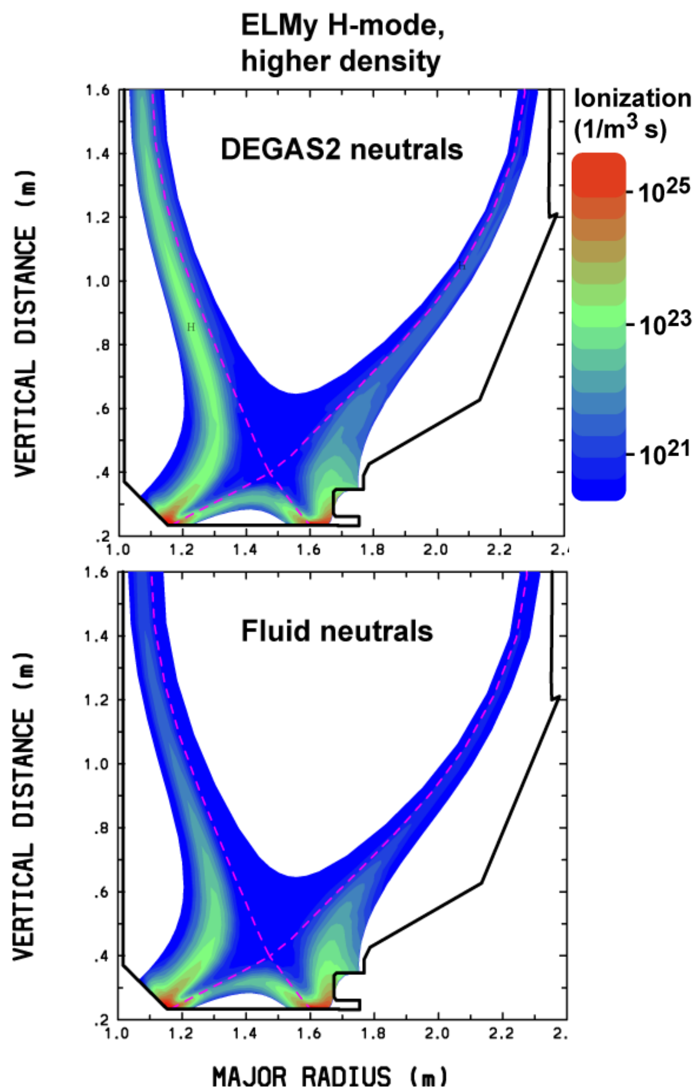


The fix: plasma equations utilize domain block Jacobian with some overlap during inversion; neutrals are global

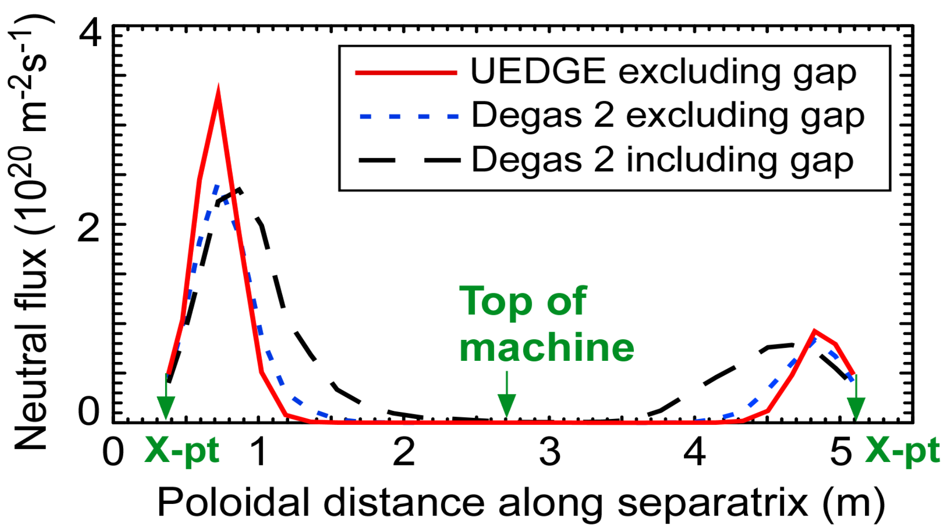
Neutral equations are placed at the end of variable list for global domain, and J_N is inverted on global domain

$$\underbrace{\begin{pmatrix} \left.\begin{bmatrix} (n_\mathrm{i})_1 \\ (m_\mathrm{i} v_\parallel)_1 \\ (T_\mathrm{i})_1 \\ (T_\mathrm{e})_1 \\ \vdots \\ (n_\mathrm{i})_M \\ (m_\mathrm{i} v_\parallel)_M \\ (T_\mathrm{i})_M \\ (T_\mathrm{e})_M \end{bmatrix}\right\} \mathbf{u}_P \\ \left.\begin{bmatrix} (n_\mathrm{n})_1 \\ \vdots \\ (n_\mathrm{n})_N \end{bmatrix}\right\} \mathbf{u}_N \end{pmatrix}}_{\text{unknowns}} \qquad \underbrace{\begin{pmatrix} \begin{bmatrix} \mathsf{J}_P(F)(\mathbf{u}_P) \end{bmatrix} & \begin{bmatrix} \mathsf{J}_P(F)(\mathbf{u}_N) \end{bmatrix} \\ \begin{bmatrix} \mathsf{J}_N(F)(\mathbf{u}_P) \end{bmatrix} & \begin{bmatrix} \mathsf{J}_N(F)(\mathbf{u}_N) \end{bmatrix} \end{pmatrix}}_{\text{Jacobian}},$$

Issue: how do of fluid and Monte Carlo neutral compare?



- **Fixed plasma conditions with fluid using flux limits**
- **Main difference is some leakage of neutrals in "gap" region where plasma properties assumed**



Conclusions

1. Neutrals and impurities are generally trace-level components at the separatrix, but not necessarily near divertor plates

2. Direct impact of neutrals/impurities on microinstabilities is likely small, but turbulence has strong effect on impurity transport

3. Fluid neutral/impurity models fit naturally into present BOUT++ framework, but preconditioning for efficiently can be challenging. Coupling fluid plasma with particle-based neutrals (& impurities) allows kinetic effects but coupling may be numerically challenging.